

3,6-Diacetylmorphine
561-27-3 | DTXSID6046761

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 379 °C

Global applicability domain: Outside

Local applicability domain index: 2.64e-01

Confidence level: 5.70e-01

Nearest Neighbors from the Training Set

Image not found

Parathion

Measured: 375

Predicted: 362

Image not found

Tribenzylamine

Measured: 385

Predicted: 366

Image not found

2-Ethylhexyl diphenyl phosphate

Measured: 375

Predicted: 369

Image not found

Triphenyl phosphite

Measured: 360

Predicted: 403